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### **Swiss Science Concentrates**

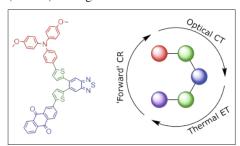
**A CHIMIA Column** 

Short Abstracts of Interesting Recent Publications of Swiss Origin

#### Circular Photoinduced Electron Transfer in a Donor-Acceptor-Acceptor Triad

Christopher B. Larsen\* and Oliver S. Wenger\*, *Angew. Chem. Int. Ed.* **2018**, *57*, 841. University of Basel

Single-molecule electronics represent the ultimate miniaturization of electrical devices. However, previous development was limited to molecules that act as individual components such as wires, switches, or rectifiers. Larsen and Wenger developed an electron-donor-acceptor-acceptor (D-A<sub>1</sub>-A<sub>2</sub>) triad as the first proof-of-concept for a single-molecule, photoinitiated molecular circuit. Circular electron transfer starts with optical charge-transfer between a triarylamine donor (D) and benzothiadiazole acceptor (A<sub>1</sub>), followed by thermal electron-transfer to a secondary anthraquinone acceptor (A<sub>2</sub>) and geometric rearrangement giving an intramolecular ion-pair D<sup>+</sup>-A<sub>1</sub>-A<sub>2</sub><sup>-</sup> in close proximity (~2.4 Å). Charge-recombination between A<sub>2</sub><sup>-</sup> and D<sup>+</sup> completes



the circuit with a quantum efficiency of ~4%. Further optimization and development of this concept may enable specific functions in future electronic and magnetic devices.

# A High-throughput Screening Method for the Crystallization of Organic Cations

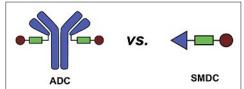
Philipp P. Nievergelt, Martin Babor, Jan Čejka, and Bernhard Spingler\*, *Chem. Sci.* **2018**, 8, DOI: 10.1039/c8sc00783g, University of Zurich

The extremely successful approach of growing protein crystals by vapor diffusion was applied to the high-throughout crystallization of small molecules. For this purpose, a screen was developed containing 77 different anions at optimized concentrations. Robots used in protein crystal screening were used to apply a mere 12 microliters of each test compound under 96 different conditions. The crystals obtained by this method were often suitable for direct, single crystal analysis. In a series of test compounds, six out of seven yielded at least one crystal structure. This approach is expected to be of great help to chemists, material scientists, and pharmacists – since it also serves as an attractive screening platform for the formulation of charged, active pharmaceutical ingredients (APIs).



### Chemically Defined Antibody-Drug Conjugates for in vivo Tumor Targeting: A Comparative Analysis

Samuele Cazzamalli, Alberto Dal Corso, Fontaine Widmayer, and Dario Neri\*, *J. Am. Chem. Soc.* **2018**, *140*, 1617. ETH Zurich One of the most critical challenges to modern chemotherapeutics is the site-specific targeting of tumors *in vivo*. The conjugation of chemotherapeutic and/or imaging agents to a delivery vehicle such as an antibody is one important way of achieving this goal. In this paper, Cazzamalli, Dal Corso, Widmayer, and Neri report the first direct comparison of chemically defined antibody-drug conjugates (ADCs) and small molecule-drug conjugates (SMDCs) directed to the same cellular target, Carbonic anhydrase IX. This membrane protein is overexpressed during tumor hypoxia and by wide variety of malignant cells. Their results demonstrate both



ADCs and SMDCs can mediate potent antitumor effects in tumor-bearing mice, even when applied at similar doses.

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## Synthetic Fermentation of $\beta$ -Peptide Macrocycles by Thiadiazole-Forming Ring-Closing Reactions

Jonathan G. Hubert, Iain A. Stepek, Hidetoshi Noda, and Jeffrey W. Bode\*, *Chem. Sci.* **2018**, *9*, 2159. ETH Zurich

A facile and efficient method for the synthesis of highly functionalized  $\beta\text{-peptide}$  macrocycles has been introduced by the group of J. W. Bode. Their strategy utilizes  $\alpha\text{-ketoacid-hydroxylamine}$  (KAHA) ligations with a bifunctional initiator – a process termed 'synthetic fermentation' in analogy to the production of natural product-like molecules from simpler building blocks. Three-component ring closing reactions included a novel oxidative coupling between  $\alpha\text{-ketoacids}$  and thiohydrazides to give 1,3,4-thiadiazoles under mild conditions. This approach does not require additional catalysts or reagents and should therefore facilitate direct biological evaluation of  $\beta\text{-peptide}$  macrocycles – a relatively underexplored class of compounds with promising biological properties.

